Exact asymptotics of monomer-dimer model on rectangular semi-infinite lattices

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By using the asymptotic theory of Pemantle and Wilson, exact asymptotic expansions of the free energy of the monomer-dimer model on rectangular $n \times \infty$ lattices in terms of dimer density are obtained for small values of n, at both high and low dimer density limits. In the high dimer density limit, the theoretical results confirm the dependence of the free energy on the parity of n, a result obtained previously by computational methods. In the low dimer density limit, the free energy on a cylinder $n \times \infty$ lattice strip has exactly the same first n terms in the series expansion as that of infinite $\infty \times \infty$ lattice.

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I. INTRODUCTION

In the previous investigation of the monomer-dimer model on two-dimensional rectangular lattices by computational methods, it is found that at high dimer density, the free energy depends on the parity of the width of the lattice strip (for a review of monomer-dimer model, see Ref. 1, 2 and references cited therein). For a $m \times n$ lattice, we define the dimer density ρ as $\rho = 2s/mn$, where s is the number of dimers. With this definition, a close-packed lattice will have $\rho = 1$. The grand canonical partition function of the monomer-dimer system in a $m \times n$ two-dimensional lattice is

$$Z_{m,n}(x) = \sum_{s=0}^{N} a_s(m,n) x^s = \sum_{0 \le \rho \le 1} a_{m,n}(\rho) x^{mn\rho/2} \quad (1)$$

where $a_s(m,n)$ is the number of distinct ways to arrange s dimers on the $m \times n$ lattice, $a_{m,n}(\rho)$ is the corresponding number at the fixed dimer density ρ, x is the activity of the dimer, and N is the maximum possible dimer on the lattice: $N = \lfloor mn/2 \rfloor$. The free energy per lattice site at a given dimer density ρ is defined as

$$f_{m,n}(\rho) = \frac{\ln a_{m,n}(\rho)}{mn}.$$

For a semi-infinite $\infty \times n$ lattice at high dimer density limit ($\rho \to 1$), the computational method shows that the free energy $f_{\infty,n}(\rho)$ depends on the parity of the lattice width n [2]:

$$f_{\infty,n}(\rho) \sim f^{\text{lattice}}_{\infty,n}(1) - \begin{cases} (1-\rho)\ln(1-\rho) & n \text{ is odd} \\ \frac{1}{2}(1-\rho)\ln(1-\rho) & n \text{ is even} \end{cases} \quad (2)$$

where $f^{\text{lattice}}_{\infty,n}(1)$ is the free energy of close-packed lattice with width n, the exact expression of which is known and is dependent on the boundary conditions of the lattice (cylinder or with free edges) [3, 4]. A slightly more general expression, for a finite $m \times n$ lattice at high dimer density limit as $\rho \to 1$ and $m \to \infty$, is given by [2]

$$f_{m,n}(\rho) \sim f^{\text{lattice}}_{\infty,n}(1) - \left\{ \begin{array}{l} (1-\rho)\ln(1-\rho) \\ \frac{1}{2}(1-\rho)\ln(1-\rho) \end{array} \right. - \frac{1}{2mn}\ln m - \frac{1}{2mn}\ln(1-\rho) \quad \begin{array}{l} n \text{ is odd} \\ n \text{ is even} \end{array} \quad (3)$$

For the coefficient of the term $(1-\rho)\ln(1-\rho)$ in the above expansion of the free energy $f_{\infty,n}(\rho)$, computational results give values very close to the value -1 when n is odd, and $-1/2$ when n is even. Although these numerical evidences strongly support the coefficients of the parity-depending term $(1-\rho)\ln(1-\rho)$ as shown in Eq. (3), there still exists slight possibility that the observations be explained in another way. This is mainly due to the following two reasons. Firstly, the sequence of n used in the computational studies is not very long. For cylinder lattices, the largest n used is 17. For lattices with free edges, maximum value of $n = 16$ is used. Secondly, at high dimer density limit, the convergent rate is the poorest and some heuristic weighting averages had to be used in the fitting procedure [2]. Due to these uncertainties, it might be possible that the different coefficients observed for these small number of even and odd lattice widths are just the initial values of two slowly changing

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sequences. When the lattice width n is small, the deviation of the coefficient from -1 or $-1/2$ is so small that it could not be detected numerically. As n becomes bigger, these two sequences might converge to some intermediate values between -1 and $-1/2$.

In this report, we use the asymptotic theory of Pemantle and Wilson [5] to get exact asymptotics for the free energy $f_{\infty,n}(\rho)$ of $n\times\infty$ lattices. The exact asymptotics show that the coefficients of $(1-\rho)\ln(1-\rho)$ in the high dimer density expansion of $f_{\infty,n}(\rho)$ is exactly -1 when n is odd, and $-1/2$ when n is even. Furthermore, the Pemantle and Wilson method is also used to investigate the low dimer density expansion of $f_{\infty,n}(\rho)$. In the low dimer density limit, the free energy on a cylinder $n\times\infty$ lattice has exactly the same first n terms as that of infinite $\infty\times\infty$ lattice. In addition, closed form expressions can be obtained for the differences of the coefficients between finite and infinite lattices of the next two terms [Eq. (15) and Table I]. These properties not only explain the fast convergence rate of the free energy on cylinder lattices when dimer density is low, but also provide a quantitative indicator of the errors when the results of finite size lattices are used to approximate the infinite lattice.

The article is organized as follows. In Section II, the Pemantle and Wilson (PW) method for asymptotics of multivariate generating functions is summarized. The starting point for the PW method is the multivariate generating function of the model under study, and in our case of the monomer-dimer model, the generating functions are bivariate. In Appendix, the bivariate generating functions of monomer-dimer models in two-dimensional rectangular lattices are listed for small values of n. These generating functions are used as the input to the PW method in this article. In Section III, the exact asymptotic expansions of $f_{\infty,n}(\rho)$ at high dimer density is derived for some small values of n. The coefficients obtained for the $(1-\rho)\ln(1-\rho)$ term confirm the dependence on the parity of n, as shown in Eq. (3). In Section IV, we discuss the exact asymptotic expansions of $f_{\infty,n}(\rho)$ at low dimer density.

II. PEMANTLE AND WILSON METHOD FOR ASYMPTOTICS OF MULTIVARIATE GENERATING FUNCTIONS

To extract asymptotics from a sequence, it's usually useful to utilize its associated generating function. The method for extract asymptotics from *univariate* generating function is well-known [6]. For multivariate generating functions, however, the techniques were "almost entirely missing" until the recent development of the Pemantle and Wilson method [5]. For combinatorial problems with known generating functions, the method can be applied in a systematic way. The theory applies to generating functions with multiple variables, and for the bivariate case that we are interested here, the generating function of two variables takes the form

$$G(x,y)=\frac{F(x,y)}{H(x,y)}=\sum_{s,m=0}^{\infty}a_{sm}x^sy^m \tag{4}$$

where $F(x,y)$ and $H(x,y)$ are analytic, and $H(0,0)\neq 0$. In this case, PW method gives the asymptotic expression as

$$a_{sm}\sim\frac{F(x_0,y_0)}{\sqrt{2\pi}}x_0^{-s}y_0^{-m}\sqrt{\frac{-y_0H_y(x_0,y_0)}{mQ(x_0,y_0)}} \tag{5}$$

where (x_0,y_0) is the positive solution to the two equations

$$H(x,y)=0,\qquad mx\frac{\partial H}{\partial x}=sy\frac{\partial H}{\partial y} \tag{6}$$

and $Q(x,y)$ is defined as

$$\begin{aligned}Q(x,y)=&-(xH_x)(yH_y)^2-(yH_y)(xH_x)^2\\&-[(yH_y)^2(x^2H_{xx})+(xH_x)^2(y^2H_{yy})\\&-2(xH_x)(yH_y)(xyH_{xy})].\end{aligned}$$

Here H_x, H_y, etc. are partial derivatives $\partial H/\partial x$, $\partial H/\partial y$, and so on. One of the advantages of the method over previous ones is that the convergence of Eq. (5) is *uniform* when s/m and m/s are bounded.

For the monomer-dimer model discussed here, with n as the finite width of the lattice strip, m as the length, and s as the number of dimers, we can construct the bivariate generating function $G_n(x,y)$ as

$$G_n(x,y)=\sum_{m=0}^{\infty}\sum_{s=0}^{mn/2}a_s(m,n)x^sy^m=\sum_{m=0}^{\infty}Z_{m,n}(x)y^m. \tag{7}$$

For the monomer-dimer model, as well as a large class of lattice models in statistical physics, the bivariate generating function $G(x,y)$ is always in the form of Eq. (4), with $F(x,y)$ and $H(x,y)$ as polynomials in x and y. In fact, for monomer-dimer model as well as other lattice models, we can get $H(x,y)$ directly from matrix M_n used in the recursive formula to calculate the partition functions [2, 7, 8, 9]

$$\Omega_m=M_n\Omega_{m-1}.$$

Here the vector Ω_m consists of the partition function Eq. (1) as well as other contracted partition functions [7]. The function $H(x,y)$ is closely related to the characteristic function of M_n [7]: $H(x,y)=\det(M_n-I/y)\times y^w$, where w is the size of the matrix M_n. More discussions can be found in the Appendix.

The relation between the number of dimers s and the dimer density ρ is given by $s=\rho mn/2$. If we fix the dimer density ρ, and substitute this relation into Eq. (6), then we see that the solution (x_0,y_0) of Eq. (6) depends only on ρ and n, and does not depend on m or s:

$$\begin{aligned}&H(x,y)=0,\\&x\frac{\partial H}{\partial x}=\frac{\rho ny}{2}\frac{\partial H}{\partial y}.\end{aligned} \tag{8}$$

Substituting this solution $(x_0(n,\rho), y_0(n,\rho))$ into Eq. (5) we obtain

$$f_{m,n}(\rho) \sim -\frac{1}{n}\ln(x_0^{\rho n/2}y_0) - \frac{1}{2}\frac{\ln m}{mn} + \frac{1}{mn}\ln\left(F(x_0,y_0)\sqrt{\frac{-y_0 H_y(x_0,y_0)}{2\pi Q(x_0,y_0)}}\right). \quad (9)$$

From this asymptotic expansion we obtain the logarithmic correction term with coefficient of exactly $-1/2$ (the second term in Eq. (9)), for both even and odd values of n. In fact, the PW asymptotic theory predicts that there exists such a logarithmic correction term with a coefficient of $-1/2$ for a large class of lattice models when the two variables involved are proportional, that is, when the models are at a fixed "density". For those lattice models which can be described by bivariate generating functions, this logarithmic correction term with a coefficient of $-1/2$ is universal when those models are at fixed "density". For the monomer-dimer model, this proportional relation is for s and m with $s = \rho mn/2$.

When the dimer density ρ and the lattice width n are fixed, the first term of Eq. (9) is a constant and does not depend on m. We identify it as $f_{\infty,n}(\rho)$

$$f_{\infty,n}(\rho) = -\frac{1}{n}\ln(x_0^{\rho n/2}y_0). \quad (10)$$

In theory, as long as the bivariate generating function $G(x,y)$ or its denominator $H(x,y)$ is known, $(x_0,\ y_0)$ could be solved from the system of equations Eq. (8) and $f_{\infty,n}(\rho)$ could be obtained from Eq. (10). In practice, however, only very small values of n can be handled this way. When $n=1$, x_0 and y_0 can be solved as

$$x_0 = \frac{\rho(2-\rho)}{4(1-\rho)^2}, \qquad y_0 = \frac{2(1-\rho)}{2-p}$$

which leads to

$$f_{\infty,1}(\rho) = (1-\frac{\rho}{2})\ln(1-\frac{\rho}{2}) - \frac{\rho}{2}\ln\frac{\rho}{2} - (1-\rho)\ln(1-\rho).$$

This expression is exact for $0 \le \rho \le 1$.

When $n=2$, for both the cylinder lattice and the lattice with free boundaries, $H(x,y)$ is a cubic polynomial (Appendix). From Eq. (8) a quartic equation can be obtained for x_0. For the cylinder lattice, x_0 satisfies the following quartic equation

$$32\,(1-\rho)^3\,x^4 + 144\,(1-\rho)^3\,x^3 + 4\,(1-\rho)\left(10\,\rho^2 - 20\,\rho + 3\right)x^2 + 4\,(2-\rho)\left(3\,\rho^2 - 3\,\rho + 1\right)x - \rho\,(1-\rho)\,(2-\rho) = 0. \quad (11)$$

After x_0 is solved, y_0 can be obtained as a rational function in ρ as

$$y_0 = \frac{w(x_0,\rho)}{v(\rho)} \quad (12)$$

where

$$\begin{aligned} w(x_0,\rho) = {} & \left(1440\,\rho^5 - 11424\,\rho^2 + 12960\,\rho^3 - 672 + 4672\,\rho - 6976\,\rho^4\right){x_0}^3 \\ & + \left(-3360 + 60432\,\rho^3 - 53936\,\rho^2 + 6608\,\rho^5 - 32240\,\rho^4 + 22496\,\rho\right){x_0}^2 \\ & + \left(23532\,\rho^3 - 1716 - 12072\,\rho^4 + 2288\,\rho^5 - 21240\,\rho^2 + 9208\,\rho\right)x_0 \\ & + 744\,\rho - 54 + 2812\,\rho^3 - 1552\,\rho^4 + 300\,\rho^5 - 2182\,\rho^2 \end{aligned}$$

and

$$v(\rho) = (1-\rho)\,(2-\rho)\left(43\,\rho^3 - 123\,\rho^2 + 90\,\rho - 27\right).$$

Although when $n=2$ closed form expressions could be written down for x_0 and y_0 (and hence $f_{\infty,2}(\rho)$) as a function of ρ, the long expressions are not very informative. We can, however, obtain highly accurate numerical results from Eqs. (11) and (12) for the $n=2$ cylinder lattice for different values of ρ. For example, when $\rho = 1/2$, we can solve x_0 and y_0 numerically from Eqs. (11) and (12) as $x_0 = 0.389620618156217959$ and $y_0 = 0.442004100446556690$, which lead to $f_{\infty,2}(\frac{1}{2}) = 0.643863506776659088$.

For the $n=3$ cylinder lattice, in order to solve x_0 (or y_0), we have to solve a polynomial equation with a degree of 10. When ρ is not so close to 1, reliable numerical solutions can be obtained. For example, when $\rho = 1/2$, x_0 and y_0 can be solved as 0.441361340073863149 and 0.277272018269763844 respectively, leading to $f_{\infty,3}(\frac{1}{2}) = 0.632058256526951594$. These "exact" numerical values can be used to check the results obtained previously by the computational methods (Table I, Ref. 2). This procedure confirms the conclusion that the computational methods used previously give results with up to 12 and 13 correct digits.

For bigger n, it becomes increasingly difficult to solve the system of polynomial equations Eq. (8). Even numerical solutions become highly unstable, especially at high dimer density. In the following we investigate the series expansions of the free energy for lattice strips $n\times\infty$

for small values of n. Since the behaviors of the solution x_0 and y_0, and hence the asymptotics of the free energy $f_{\infty,n}(\rho)$, are quite different at the high and the low dimer density limits, we discuss the two cases separately.

III. ASYMPTOTICS AT THE HIGH DIMER DENSITY LIMIT

For clarity we define $u = 1 - \rho$. At the high dimer density limit when $u \to 0$, numerical calculations show that for both odd and even n, $x_0 \to \infty$ and $y_0 \to 0$. If we expand $1/x_0$ and y_0 as series of u, from Eq. (8) it is found that $1/x_0$ and y_0 have different leading terms in the series expansion for odd and even n. For odd n, the leading term of $1/x_0$ is u^2 and the leading term of y_0 is u^n. For even n, the leading terms of $1/x_0$ and y_0 are u and $u^{n/2}$ respectively:

$$\frac{1}{x_0} = \sum_{i=2}^{\infty} a_i u^i, \qquad y_0 = \sum_{i=n}^{\infty} b_i u^i \qquad \text{when } n \text{ is odd}$$

$$\frac{1}{x_0} = \sum_{i=1}^{\infty} a_i u^i, \qquad y_0 = \sum_{i=n/2}^{\infty} b_i u^i \qquad \text{when } n \text{ is even.}$$

These differences in the leading terms of the series expansions of x_0 and y_0 lead directly to the different coefficients of $u \ln u$ in $f_{\infty,n}(u)$ for odd and even n. By using Eq. (10) we obtain for odd n,

$$\begin{aligned} f_{\infty,n}(u) &\sim \frac{1-u}{2}\ln(a_2u^2 + a_3u^3 + \cdots) \\ &\quad - \frac{1}{n}\ln(b_nu^n + b_{n+1}u^{n+1} + \cdots) \\ &= \left[\frac{\ln a_2}{2} - \frac{\ln b_n}{n}\right] - u\ln u \\ &\quad + \left[\frac{a_3}{2a_2} - \frac{b_{n+1}}{nb_n} - \frac{\ln a_2}{2}\right] u + \cdots \end{aligned}$$

and for even n,

$$\begin{aligned} f_{\infty,n}(u) &\sim \frac{1-u}{2}\ln(a_1u + a_2u^2 + \cdots) \\ &\quad - \frac{1}{n}\ln(b_{\frac{n}{2}}u^{\frac{n}{2}} + b_{\frac{n}{2}+1}u^{\frac{n}{2}+1} + \cdots) \\ &= \left[\frac{\ln a_1}{2} - \frac{\ln b_{\frac{n}{2}}}{n}\right] - \frac{1}{2}u\ln u \\ &\quad + \left[\frac{a_2}{2a_1} - \frac{b_{\frac{n}{2}+1}}{nb_{\frac{n}{2}}} - \frac{\ln a_1}{2}\right] u + \cdots \end{aligned}$$

The difference in the coefficients of $u \ln u$ in $f_{\infty,n}(u)$ comes directly from the different leading terms of $1/x_0$ for odd and even n.

Some explicit expressions of $f_{\infty,n}(\rho)$ for cylinder lattices and lattices with free boundaries are listed in the following.

A. Cylinder lattices

The asymptotic expansions of $f_{\infty,n}(\rho)$ in cylinder lattices at the high dimer density are listed below for $n = 1, \ldots, 5$. For cylinder lattices, the constant term of $f_{\infty,n}(\rho)$ is given by the following exact expression [3]

$$f_{\infty,n}(1) = \frac{1}{n}\ln\prod_{i=1}^{n/2}\left[\sin\frac{(2i-1)\pi}{n} + \left(1+\sin^2\frac{(2i-1)\pi}{n}\right)^{\frac{1}{2}}\right],$$

which can be used to check the constant terms in the following results.

For $n = 1$,

$$f_{\infty,1}(u) \sim -u\ln u - (\ln 2 - 1)u - \sum_{i=1}^{\infty}\frac{u^{2i+1}}{2i(2i+1)}.$$

For $n = 2$,

$$\begin{aligned} f_{\infty,2}(u) \sim{}& \frac{1}{2}\ln\left(1+\sqrt{2}\right) - \frac{1}{2}u\ln(u) \\ &+ \frac{1}{2}\left[1 - \ln\left(4 - 2\sqrt{2}\right)\right]u \\ &- \left[\frac{1}{2} + \frac{1}{8}\sqrt{2}\right]u^2 - \left[\frac{1}{3} - \frac{1}{8}\sqrt{2}\right]u^3 \\ &- \left[\frac{1}{3} - \frac{67}{192}\sqrt{2}\right]u^4 - \left[\frac{9}{10} - \frac{45}{64}\sqrt{2}\right]u^5 \\ &- \left[\frac{38}{15} - \frac{6077}{3840}\sqrt{2}\right]u^6 \\ &- \left[\frac{142}{21} - \frac{1169}{256}\sqrt{2}\right]u^7 \end{aligned}$$

For $n = 3$,

$$\begin{aligned} f_{\infty,3}(u) \sim{}& \frac{1}{6}\ln\left(\frac{5}{2} + \frac{1}{2}\sqrt{21}\right) - u\ln(u) \\ &+ \left[1 - \frac{1}{2}\ln\left(\frac{6300}{289} - \frac{1008}{289}\sqrt{21}\right)\right]u \\ &- \left[\frac{96}{289} - \frac{200}{2023}\sqrt{21}\right]u^2 \\ &- \left[\frac{1975875}{167042} - \frac{1368324}{584647}\sqrt{21}\right]u^3 \\ &- \left[\frac{2500298208}{24137569} - \frac{27592174000}{1182740881}\sqrt{21}\right]u^4 \end{aligned}$$

For $n = 4$,

$$\begin{aligned} f_{\infty,4}(u) \sim{}& -\frac{1}{4}\ln\left(2 - \sqrt{3}\right) - \frac{1}{2}u\ln(u) \\ &+ \frac{1}{2}\left[1 - \ln\left(\frac{102}{23} - \frac{54}{23}\sqrt{3}\right)\right]u \\ &- \left[\frac{1008}{529} + \frac{149}{1058}\sqrt{3}\right]u^2 \\ &- \left[\frac{6535949}{839523} - \frac{2581941}{559682}\sqrt{3}\right]u^3 \\ &- \left[-\frac{18405319107}{148035889} - \frac{23448085573}{296071778}\sqrt{3}\right]u^4 \end{aligned}$$

For $n = 5$,

$$f_{\infty,5}(u) \sim \frac{1}{5} \ln \frac{\sqrt{5}+\sqrt{41}+\sqrt{15-2\sqrt{5}}+\sqrt{5+2\sqrt{5}}}{4} - u \ln(u) + \left[1 + \frac{1}{2} \ln \frac{849+44\sqrt{205}+12\sqrt{6215+422\sqrt{205}}}{20500}\right] u.$$

B. Lattices with free boundaries

The asymptotic expansions of $f_{\infty,n}(\rho)$ in lattices with free boundaries at the high dimer density are listed below for $n = 1, \ldots, 4$. For lattices with free boundaries, the constant term of $f_{\infty,n}(\rho)$ is given by the following exact expression [3]

$$f^{\rm fb}_{\infty,n}(1) = \frac{1}{n} \ln \left[\prod_{i=1}^{\frac{n}{2}} \left(\cos \frac{i\pi}{n+1} + \left(1 + \cos^2 \frac{i\pi}{n+1}\right)^{\frac{1}{2}} \right) \right],$$

which can be used to check the constant terms of the following results.

For $n = 2$,

$$\begin{aligned} f^{\rm fb}_{\infty,2}(u) \sim& \frac{1}{2} \ln \left(\frac{1}{2} + \frac{1}{2}\sqrt{5} \right) - \frac{1}{2} u \ln(u) \\ &+ \frac{1}{2}\left[1 - \ln\left(5 - 2\sqrt{5}\right)\right] u \\ &- \left[1 + \frac{1}{20}\sqrt{5}\right] u^2 + \left[\frac{2}{5}\sqrt{5} - \frac{13}{12}\right] u^3 \\ &+ \left[-\frac{8}{3} + \frac{1073}{600}\sqrt{5}\right] u^4 + \left[\frac{162}{25}\sqrt{5} - \frac{561}{40}\right] u^5 \\ &+ \left[\frac{221359}{7500}\sqrt{5} - \frac{1096}{15}\right] u^6 \\ &- \left[\frac{31249}{84} - \frac{20564}{125}\sqrt{5}\right] u^7 \end{aligned}$$

For $n = 3$,

$$\begin{aligned} f^{\rm fb}_{\infty,3}(u) \sim& \frac{1}{6} \ln\left(2 + \sqrt{3}\right) - u \ln(u) \\ &+ \left[1 + \ln\left(\frac{1}{36}\sqrt{6} + \frac{1}{6}\sqrt{2}\right)\right] u \\ &+ \left[\frac{103}{121}\sqrt{3} + \frac{240}{121}\right] u^2 \\ &- \left[\frac{112740}{14641}\sqrt{3} + \frac{806673}{29282}\right] u^3 \\ &+ \left[\frac{369777941}{1771561}\sqrt{3} + \frac{492403464}{1771561}\right] u^4 \\ &- \left[\frac{30323479269681}{4287177620} + \frac{662980595688}{214358881}\sqrt{3}\right] u^5 \end{aligned}$$

For $n = 4$,

$$\begin{aligned} f^{\rm fb}_{\infty,4}(u) \sim& \frac{1}{4} \ln \frac{\sqrt{5}+1+\sqrt{22+2\sqrt{5}}}{4} \\ &+ \frac{1}{4} \ln \frac{\sqrt{5}-1+\sqrt{22-2\sqrt{5}}}{4} \\ &- \frac{1}{2} u \ln(u) \\ &+ \Bigg[\frac{1}{2} + \frac{1}{2} \ln \frac{341801}{2} \\ &\quad - \frac{1}{2} \ln\Big(545403 + 81734\sqrt{29} \\ &\quad - 4\sqrt{27680943526 + 5123717738\sqrt{29}}\Big)\Bigg] u. \end{aligned}$$

IV. ASYMPTOTICS AT THE LOW DIMER DENSITY LIMIT

Unlike the high dimer density case, at low dimer density when $\rho \to 0$, numerical calculations show that x_0 approaches zero and y_0 approaches 1, for both odd and even values of n. The series expansions of x_0 and y_0 thus have the following forms:

$$x_0 = \sum_{i=1}^{\infty} a_i \rho^i, \qquad y_0 = 1 + \sum_{i=1}^{\infty} b_i \rho^i$$

From Eq. (10), the general form of the free energy at the low dimer density is

$$f_{\infty,n}(\rho) \sim -\frac{\rho \ln \rho}{2} - \left[\frac{\ln a_1}{2} + \frac{b_1}{2}\right] \rho - \left[\frac{a_2}{2a_1} + \frac{b_2}{n} - \frac{b_1^2}{2n}\right] \rho^2 + \cdots$$

For both odd and even values of n, at low dimer density the coefficient of logarithmic term $\rho \ln \rho$ is $-1/2$, consistent with the previous results obtained by computational methods [9]. This coefficient comes directly from the fact that the leading term in the series expansion of x_0 is $a_1 \rho$.

The asymptotic expansions of free energy in cylinder lattices at low dimer density show an interesting property: for lattice strip $n \times \infty$ with a width of n, the first n terms in the series expansion of $f_{\infty,n}(\rho)$ is exactly the same as the first n terms in the series expansion of $f_{\infty,\infty}(\rho)$, the free energy of the infinite lattice. In order to compare the free energy in semi-infinite $n \times \infty$ lattice strips with that of an infinite $\infty \times \infty$ lattice, in the following section the series of Gaunt [10] is used to derive the series of $f_{\infty,\infty}(\rho)$.

A. Free energy for an infinite lattice

Gaunt gave a series expansion of the dimer activity x as a function of the number density t (Ref. 10, column 2

of Table II):

$$\begin{aligned} x(t) = & t + 7\,t^2 + 40\,t^3 + 206\,t^4 + 1000\,t^5 \\ & + 4678\,t^6 + 21336\,t^7 + 95514\,t^8 \\ & + 421472\,t^9 + 1838680\,t^{10} + 7947692\,t^{11} \\ & + 34097202\,t^{12} + 145387044\,t^{13} \\ & + 616771148\,t^{14} + 2605407492\,t^{15} + \cdots . \end{aligned} \tag{13}$$

Here $t = \theta/4$, where θ is the average number of sites covered by dimers when grand canonical ensembles are considered [2].

By using the relation between the grand canonical ensemble and the canonical ensemble [2] and identifying θ with the dimer density ρ, we have the following relation

$$f_{\infty,\infty}(\rho) = -\frac{1}{2}\int \ln\left[x\left(\frac{\rho}{4}\right)\right] d\rho.$$

From this relation and the series in Eq. (13) we can obtain the series expression for the free energy of the infinite lattice

$$\begin{aligned} f_{\infty,\infty}(\rho) = & -\frac{1}{2}\,\rho\ln(\rho) + \left[\frac{1}{2} + \ln(2)\right]\rho - \frac{7}{16}\,\rho^2 \\ & - \frac{31}{192}\,\rho^3 - \frac{121}{1536}\,\rho^4 - \frac{471}{10240}\,\rho^5 \\ & - \frac{1867}{61440}\,\rho^6 - \frac{7435}{344064}\,\rho^7 - \frac{4211}{262144}\,\rho^8 \\ & - \frac{116383}{9437184}\,\rho^9 - \frac{459517}{47185920}\,\rho^{10} - \frac{1821051}{230686720}\,\rho^{11} \\ & - \frac{7255915}{1107296256}\,\rho^{12} - \frac{9687973}{1744830464}\,\rho^{13} \\ & - \frac{16697149}{3489660928}\,\rho^{14} \\ & - \frac{157001097}{37580963840}\,\rho^{15} + \cdots . \end{aligned} \tag{14}$$

B. Cylinder lattices

The coefficients of ρ^i in the series expansion of $f_{\infty,n}(\rho)$ at low dimer density is listed in Table I for $n = 1, \ldots, 7$. The term $-\frac{1}{2}\rho\ln(\rho)$, which is common to lattices of all sizes, is not included in the Table. Also listed in the last row of the Table are the coefficients for the infinite lattice (Eq. (14)). It is evident from the Table that for lattice strip $n\times\infty$ with a width of n, the first n terms of $f_{\infty,n}(\rho)$ (including the term of $-\frac{1}{2}\rho\ln(\rho)$) is exactly the same as the first n terms of the infinite lattice $f_{\infty,\infty}(\rho)$. For example, the lattice strip $7\times\infty$ has the first seven terms identical to those of the infinite lattice, up to the term of ρ^6. This nice property gives a quantitative estimate of the error when we use the values of finite lattices to approximate the properties of the infinite lattice. It also explains why the sequence of the free energy in cylinder lattices converges so fast, especially when ρ is small [2].

The term of ρ^n in $f_{\infty,n}(\rho)$ is the first term that differs from the series expansion of $f_{\infty,\infty}(\rho)$. The difference between the coefficients of ρ^n in $f_{\infty,n}(\rho)$ and $f_{\infty,\infty}(\rho)$ shows a regular pattern: starting from $n = 2$, the differences are $\frac{1}{32}, -\frac{1}{192}, \frac{1}{1024}, -\frac{1}{5120}, \frac{1}{24576}, -\frac{1}{114688}, \ldots$. For example, for $n = 2$, $-\frac{13}{32} - (-\frac{7}{16}) = \frac{1}{32}$. The closed form of this alternating sequences clearly is $\frac{(-1)^n}{n4^n}$.

The difference between the coefficients of ρ^{n+1}, the second term that differs between finite and infinite lattices, also shows a regular pattern. Starting from $n = 3$, the sequence is $-\frac{1}{256}, \frac{1}{1024}, -\frac{1}{4096}, \frac{1}{16384}, -\frac{1}{65536}, \ldots$. It is obvious that the sequence takes the closed form expression $\frac{(-1)^n}{4\cdot 4^n}$. Due to the limited number of data points in Table I, currently it is not clear whether the differences of higher degree terms also can be written in simple closed forms.

From the closed form expressions of these two dominant terms that differ between finite and infinite lattices at low dimer density, we see that when $n \geq 3$

$$f_{\infty,\infty}(\rho) \sim f_{\infty,n}(\rho) - \frac{(-1)^n}{4^n}\left(\frac{\rho^n}{n} + \frac{\rho^{n+1}}{4}\right) + O(\rho^{n+2}). \tag{15}$$

The coefficients of ρ^i in the series expansion of x_0 and $-(\ln y_0)/n$ are also listed in Tables II and III. From the Tables we can see that for cylinder lattice strips $n\times\infty$, x_0 and $(\ln y_0)/n$ share the same first $n-1$ terms with their corresponding series expansions of the infinite lattice.

C. Lattices with free boundaries

The coefficients of ρ^i in the series expansion of $f_{\infty,n}(\rho)$ for lattices with free boundaries at low dimer density is listed in Table IV for $n = 2, 3$, and 4. The term $-\frac{1}{2}\rho\ln(\rho)$, which is common to lattices of all sizes, is not included in the Table. From the Table we can see that, unlike cylinder lattices, none of the coefficients is the same as the coefficients of the infinite lattice.

As for the cylinder lattices, the coefficients of ρ^i in the series expansion of x_0 and $-(\ln y_0)/n$ are also listed in Tables V and VI. Again, except for the coefficient of ρ in $(\ln y_0)/n$, none of the coefficients is the same as the coefficients of the infinite lattice.

APPENDIX A: BIVARIATE GENERATING FUNCTIONS OF MONOMER-DIMER MODELS IN TWO-DIMENSIONAL PLANAR LATTICES

The bivariate generating functions of monomer-dimer models can be derived directly from the matrices M_n which are used in the computational studies [2, 7, 8, 9]. The denominator $H(x, y)$ of the bivariate generating functions $G(x, y)$ is directly related to the characteristic function of M_n:

$$H(x, y) = \det(M_n - y^{-1}I) \times y^w,$$

where w is the size of the matrix M_n. For the purpose of this article, it is sufficient to know the information

TABLE I: Coefficients of ρ^i in the series expansion of $f_{\infty,n}(\rho)$ of cylinder lattices at low dimer density. The term $-\frac{1}{2}\rho\ln(\rho)$, common to lattices of all sizes, is not shown. The last row for the infinite lattice $f_{\infty,\infty}(\rho)$ is taken from the series expansion Eq. (14). Terms of $f_{\infty,n}(\rho)$ that are equal to those of the infinite lattice are underlined.

n	ρ	$-\rho^2$	$-\rho^3$	$-\rho^4$	$-\rho^5$	$-\rho^6$	$-\rho^7$	$-\rho^8$
1	$\frac{\ln 2+1}{2}$	3/8	7/48	5/64	31/640	21/640	127/5376	255/14336
2	$\ln 2 + 1/2$	13/32	115/768	419/6144	5491/163840	17489/983040	116687/11010048	423771/58720256
3	$\ln 2 + 1/2$	7/16	1/6	127/1536	1027/20480	8653/245760	17677/688128	2381/131072
4	$\ln 2 + 1/2$	7/16	31/192	239/3072	461/10240	3569/122880	27325/1376256	7579/524288
5	$\ln 2 + 1/2$	7/16	31/192	121/1536	473/10240	941/30720	3791/172032	4375/262144
6	$\ln 2 + 1/2$	7/16	31/192	121/1536	471/10240	1243/40960	3707/172032	4177/262144
7	$\ln 2 + 1/2$	7/16	31/192	121/1536	471/10240	1867/61440	3719/172032	4215/262144
∞	$\ln 2 + 1/2$	7/16	31/192	121/1536	471/10240	1867/61440	7435/344064	4211/262144

TABLE II: The coefficients in the series expansion of x_0 for cylinder lattice strips $n \times \infty$ at low dimer density. Terms that are equal to those of the infinite lattice are underlined.

n	ρ	ρ^2	ρ^3	ρ^4	ρ^5	ρ^6	ρ^7	ρ^8
1	1/2	3/4	1	5/4	3/2	7/4	2	9/4
2	1/4	13/32	71/128	1393/2048	6353/8192	55073/65536	230343/262144	7519577/8388608
3	1/4	7/16	81/128	423/512	4179/4096	9993/8192	23341/16384	854147/524288
4	1/4	7/16	5/8	411/512	497/512	289/256	20917/16384	370861/262144
5	1/4	7/16	5/8	103/128	2001/2048	9369/8192	42803/32768	192145/131072
6	1/4	7/16	5/8	103/128	125/128	9355/8192	21329/16384	190871/131072
7	1/4	7/16	5/8	103/128	125/128	2339/2048	42673/32768	191043/131072
∞	1/4	7/16	5/8	103/128	125/128	2339/2048		

TABLE III: The coefficients in the series expansion of $-\ln(y_0)/n$ for cylinder lattice strips $n \times \infty$ at low dimer density. Terms that are equal to those of the infinite lattice are underlined.

n	ρ	ρ^2	ρ^3	ρ^4	ρ^5	ρ^6	ρ^7	ρ^8
1	1/2	3/8	7/24	15/64	31/160	21/128	127/896	255/2048
2	1/2	13/32	115/384	419/2048	5491/40960	17489/196608	116687/1835008	423771/8388608
3	1/2	7/16	1/3	127/512	1027/5120	8653/49152	17677/114688	16667/131072
4	1/2	7/16	31/96	239/1024	461/2560	3569/24576	27325/229376	53053/524288
5	1/2	7/16	31/96	121/512	473/2560	941/6144	3791/28672	30625/262144
6	1/2	7/16	31/96	121/512	471/2560	1243/8192	3707/28672	29239/262144
7	1/2	7/16	31/96	121/512	471/2560	1867/12288	3719/28672	29505/262144
∞	1/2	7/16	31/96	121/512	471/2560	1867/12288		

TABLE IV: Coefficients of ρ^i in the series expansion of $f_{\infty,n}(\rho)$ of lattices with free boundaries at low dimer density. The term $-\frac{1}{2}\rho\ln(\rho)$, common to lattices of all sizes, is not shown. Numbers in square brackets denote powers of 10.

n	ρ	$-\rho^2$	$-\rho^3$	$-\rho^4$	$-\rho^5$	$-\rho^6$	$-\rho^7$	$-\rho^8$
2	$\frac{1}{2}(\ln 3 + 1)$	5/12	17/108	49/648	403/9720	25/972	3223/183708	27569/2204496
3	$\frac{1}{2}(\ln(10/3) + 1)$	87/2[2]	1569/1[4]	14697/2[5]	2208627/5[7]	192832569/625[7]	9382406661/4375[8]	1278517726503/875[11]
4	$\frac{1}{2}(\ln(7/2) + 1)$	43/98	1123/7203	26323/352947	187546/4117715	18361592/605304105	850524016/41523861603	70713460952/4747561509943

TABLE V: x_0 The coefficients in the series expansion of x_0 for $n \times \infty$ lattices with free boundaries at low dimer density. Numbers in square brackets denote powers of 10.

n	ρ	ρ^2	ρ^3	ρ^4	ρ^5	ρ^6	ρ^7	ρ^8
2	1/3	5/9	7/9	239/243	851/729	2909/2187	29017/19683	31507/19683
3	3/10	261/5[2]	9207/125[2]	116397/125[3]	4826031/3125[4]	021574591/15625[5]	28645564383/1953125[4]	3178995484149/1953125[6]
4	2/7	172/343	11888/16807	738720/823543	6219872/5764801	354308800/282475249	137557926784/96889010407	7481262371584/4747561509943

TABLE VI: $-\ln(y_0)/n$ The coefficients in the series expansion of $-(\ln y_0)/n$ for $n \times \infty$ lattices with free boundaries at low dimer density. Numbers in square brackets denote powers of 10.

n	ρ	ρ^2	ρ^3	ρ^4	ρ^5	ρ^6	ρ^7	ρ^8
2	1/2	5/12	17/54	49/216	403/2430	125/972	3223/30618	27569/314928
3	1/2	87/2[2]	1569/5[3]	44091/2[5]	2208627/125[5]	192832569/125[7]	28147219983/21875[7]	1278517726503/125[11]
4	1/2	43/98	2246/7203	26323/117649	750184/4117715	18361592/121060821	1701048032/13841287201	70713460952/678223072849

of $H(x,y)$. From $H(x,y)$ and a few initial terms, the bivariate generating functions can be obtained. For completeness we list $G(x,y)$ for small values of n in this Appendix. The cylinder lattices and lattices with free edges are listed separately. Variable x is associated with the number of dimers s and variable y is associated with the length of the lattice m, as defined in Eq. (7).

When $n=1$, there is no distinction between these two boundary conditions:

$$G_1 = \frac{1}{1-y-xy^2}.$$

1. Cylinder lattices

For $n=2$,

$$G_2^c = \frac{1-yx}{1-(1+3\,x)\,y+x\,(x-1)\,y^2+y^3x^3}.$$

For $n=3$,

$$G_3^c = \frac{1-2\,yx-y^2x^3}{x^6y^4-x^3\,(x-1)\,y^3-x\,(1+3\,x+5\,x^2)\,y^2-(5\,x+1)\,y+1}.$$

For $n=4$, $G_4^c = F_4/H_4$, where

$$F_4 = -x^8y^4+3\,x^5y^3+4\,x^4y^2-x\,(3+4\,x)\,y+1,$$

and

$$\begin{aligned}H_4 =&x^{12}y^6-x^8\left(-x+2\,x^2+1\right)y^5\\&-x^5\left(6\,x^2+2\,x+1+9\,x^3\right)y^4\\&+2\,x^3\left(13\,x^2+5\,x+1+4\,x^3\right)y^3\\&+x\left(-6\,x-1+7\,x^3-6\,x^2\right)y^2\\&-(x+1)\,(6\,x+1)\,y+1.\end{aligned}$$

For $n=5$, $G_5^c = F_5/H_5$, where

$$\begin{aligned}F_5 =&-x^{15}y^6+2\,x^{11}\,(-2+x)\,y^5\\&+x^8\left(8\,x^2+2+11\,x\right)y^4\\&+2\,x^5\left(7\,x^2+3+8\,x\right)y^3\\&-x^3\left(2-x+8\,x^2\right)y^2\\&-2\,x\,(2+5\,x)\,y+1,\end{aligned}$$

and

$$\begin{aligned}H_5 =&x^{20}y^8+x^{15}\left(3\,x^2-x+1\right)y^7\\&-x^{11}\left(19\,x^4+11\,x^3+7\,x^2+2\,x+1\right)y^6\\&-x^8\left(2\,x^4+65\,x^3+39\,x^2+11\,x+2\right)y^5\\&+x^5\left(41\,x^5+95\,x^4+39\,x^3-9\,x^2-6\,x-1\right)y^4\\&+x^3\left(34\,x^4+85\,x^3+69\,x^2+19\,x+2\right)y^3\\&-x\left(19\,x^4+19\,x^3+27\,x^2+10\,x+1\right)y^2\\&-\left(15\,x^2+9\,x+1\right)y+1.\end{aligned}$$

2. Lattices with free boundaries

For $n=2$,

$$G_2^{\mathrm{fb}} = \frac{1-xy}{x^3y^3-xy^2-(2\,x+1)\,y+1}.$$

For $n=3$, $G_3^{\mathrm{fb}} = F_3^{\mathrm{fb}}/H_3^{\mathrm{fb}}$, where

$$F_3^{\mathrm{fb}} = x^6y^4+x^4y^3-2\,x^2\,(1+x)\,y^2-xy+1,$$

and

$$\begin{aligned}H_3^{\mathrm{fb}} =&-x^9y^6+x^6\,(x-1)\,y^5\\&+x^4\left(5\,x^2+3\,x+2\right)y^4+x^2\,(2\,x+1)\,(x-1)\,y^3\\&-x\,(1+x)\,(5\,x+2)\,y^2-(1+3\,x)\,y+1.\end{aligned}$$

For $n=4$, $G_4^{\mathrm{fb}} = F_4^{\mathrm{fb}}/H_4^{\mathrm{fb}}$, with

$$\begin{aligned}F_4^{\mathrm{fb}} =&x^{14}y^7-2\,x^{11}y^6-x^8\left(3\,x+5\,x^2+3\right)y^5\\&+x^6\,(2\,x+3)\,(1+x)\,y^4\\&+x^4\,(2\,x+3)\,(1+3\,x)\,y^3\\&-3\,x^2\left(1+3\,x+x^2\right)y^2\\&-2\,x\,(1+x)\,y+1,\end{aligned}$$

and

$$\begin{aligned}H_4^{\mathrm{fb}} =&-x^{18}y^9+x^{14}\left(-x+x^2+1\right)y^8\\&+x^{11}\left(2+9\,x^3+3\,x+9\,x^2\right)y^7\\&-x^8\left(19\,x^3-1+6\,x^2+5\,x^4\right)y^6\\&-x^6\left(29\,x^2+3+14\,x+24\,x^3+21\,x^4\right)y^5\\&+x^4\left(41\,x^2+40\,x^3+9\,x^4+18\,x+3\right)y^4\\&+x^2\left(4\,x^2-1-4\,x+15\,x^4+27\,x^3\right)y^3\\&-x\left(5\,x^3+2+21\,x^2+13\,x\right)y^2\\&+\left(-1-3\,x^2-5\,x\right)y+1.\end{aligned}$$

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